Table S6: List of GNPs Spectrum IDs used for Model Performance Metrics

Actinomycins:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005731085 | CCMSLIB00005731165 | CCMSLIB00005731174 | CCMSLIB00005731195 |
| CCMSLIB00005731204 | CCMSLIB00005731224 | CCMSLIB00005731230 | CCMSLIB00005731239 |
| CCMSLIB00005731385 | CCMSLIB00005731391 | CCMSLIB00005731426 | CCMSLIB00005731455 |
| CCMSLIB00005731514 | CCMSLIB00005731524 | CCMSLIB00005731578 | CCMSLIB00005731656 |
| CCMSLIB00005731663 | CCMSLIB00005731776 | CCMSLIB00005731783 | CCMSLIB00005731826 |
| CCMSLIB00005731841 | CCMSLIB00005731905 | CCMSLIB00005731964 | CCMSLIB00005732032 |
| CCMSLIB00005732084 |

Allylamines:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005732087 | CCMSLIB00005732096 | CCMSLIB00005732099 | CCMSLIB00005732127 |
| CCMSLIB00005732147 | CCMSLIB00005732182 | CCMSLIB00005732232 | CCMSLIB00005732250 |
| CCMSLIB00005732258 | CCMSLIB00005732353 | CCMSLIB00005732416 | CCMSLIB00005732457 |
| CCMSLIB00005732586 | CCMSLIB00005732777 | CCMSLIB00005732802 | CCMSLIB00005732835 |
| CCMSLIB00005732875 | CCMSLIB00005732876 | CCMSLIB00005732892 | CCMSLIB00005732936 |
| CCMSLIB00005733092 | CCMSLIB00005733180 | CCMSLIB00005733231 | CCMSLIB00005733239 |
| CCMSLIB00005733250 | CCMSLIB00005733279 | CCMSLIB00005733387 | CCMSLIB00005733413 |
| CCMSLIB00005733433 | CCMSLIB00005733454 | CCMSLIB00005733512 | CCMSLIB00005733607 |
| CCMSLIB00005733614 | CCMSLIB00005733619 | CCMSLIB00005733626 | CCMSLIB00005733787 |
| CCMSLIB00005733805 | CCMSLIB00005733807 | CCMSLIB00005733883 | CCMSLIB00005733902 |
| CCMSLIB00005734129 | CCMSLIB00005734158 | CCMSLIB00005734284 | CCMSLIB00005734304 |
| CCMSLIB00005734308 | CCMSLIB00005734330 | CCMSLIB00005734380 |

Aminocoumarins:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005734403 | CCMSLIB00005734471 | CCMSLIB00005734487 | CCMSLIB00005734496 |
| CCMSLIB00005734559 | CCMSLIB00005734641 | CCMSLIB00005734651 | CCMSLIB00005734729 |
| CCMSLIB00000005428 | CCMSLIB00005734757 | CCMSLIB00005734762 |

Aminoglycosides

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005734807 | CCMSLIB00005734844 | CCMSLIB00005734860 | CCMSLIB00005734869 |
| CCMSLIB00005734883 | CCMSLIB00005734891 | CCMSLIB00005735068 | CCMSLIB00005735088 |
| CCMSLIB00000005429 | CCMSLIB00005735162 | CCMSLIB00005735213 | CCMSLIB00005735222 |
| CCMSLIB00005735228 | CCMSLIB00005735231 | CCMSLIB00005735234 | CCMSLIB00005735250 |
| CCMSLIB00005735317 | CCMSLIB00005735330 | CCMSLIB00005735479 | CCMSLIB00000005430 |
| CCMSLIB00005735662 | CCMSLIB00005735735 | CCMSLIB00005735738 | CCMSLIB00005735758 |
| CCMSLIB00005735823 | CCMSLIB00005735835 | CCMSLIB00005735880 | CCMSLIB00005735934 |
| CCMSLIB00005735943 | CCMSLIB00005735966 | CCMSLIB00005736090 | CCMSLIB00005736109 |
| CCMSLIB00005736120 | CCMSLIB00005736302 | CCMSLIB00005736458 | CCMSLIB00005736486 |
| CCMSLIB00005736527 | CCMSLIB00000005432 | CCMSLIB00005736543 | CCMSLIB00005736585 |
| CCMSLIB00005736676 | CCMSLIB00005736698 | CCMSLIB00005736700 | CCMSLIB00005736751 |
| CCMSLIB00005753379 | CCMSLIB00005753397 | CCMSLIB00005753402 | CCMSLIB00005753464 |
| CCMSLIB00000005433 | CCMSLIB00005753543 | CCMSLIB00005753592 | CCMSLIB00005753663 |
| CCMSLIB00005753719 | CCMSLIB00005753767 | CCMSLIB00005753839 | CCMSLIB00005753848 |
| CCMSLIB00005753876 |

Ansamycins:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005753910 | CCMSLIB00000005434 | CCMSLIB00005753934 | CCMSLIB00005753968 |
| CCMSLIB00005753973 | CCMSLIB00005754003 | CCMSLIB00005754017 | CCMSLIB00005754103 |
| CCMSLIB00005754122 | CCMSLIB00005754141 | CCMSLIB00005754160 | CCMSLIB00005754193 |
| CCMSLIB00000005435 | CCMSLIB00005754211 | CCMSLIB00005754238 | CCMSLIB00005754270 |
| CCMSLIB00005754294 | CCMSLIB00005754318 | CCMSLIB00005754430 | CCMSLIB00005754443 |
| CCMSLIB00005754465 | CCMSLIB00005754500 | CCMSLIB00005754536 | CCMSLIB00000005436 |
| CCMSLIB00005754541 | CCMSLIB00005754579 | CCMSLIB00005754583 | CCMSLIB00005754672 |
| CCMSLIB00005754676 | CCMSLIB00005754686 | CCMSLIB00005754687 | CCMSLIB00005754691 |
| CCMSLIB00005754701 | CCMSLIB00005754738 | CCMSLIB00005754766 | CCMSLIB00005754775 |
| CCMSLIB00005754788 | CCMSLIB00005754797 | CCMSLIB00005754863 | CCMSLIB00005754881 |
| CCMSLIB00005754894 | CCMSLIB00005754936 | CCMSLIB00005754944 | CCMSLIB00005754959 |
| CCMSLIB00005754990 | CCMSLIB00005755035 | CCMSLIB00005755057 | CCMSLIB00005755060 |
| CCMSLIB00005755063 | CCMSLIB00005755092 | CCMSLIB00005759938 | CCMSLIB00005759961 |
| CCMSLIB00005760076 | CCMSLIB00005760338 | CCMSLIB00005760795 | CCMSLIB00005760798 |
| CCMSLIB00005761132 | CCMSLIB00005761441 | CCMSLIB00005761545 | CCMSLIB00005761737 |
| CCMSLIB00005762051 | CCMSLIB00005762701 | CCMSLIB00005762897 |

Azoles:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005776697 | CCMSLIB00005776726 | CCMSLIB00000006291 | CCMSLIB00005776864 |
| CCMSLIB00005776922 | CCMSLIB00005776923 | CCMSLIB00005777061 | CCMSLIB00005777146 |
| CCMSLIB00005777174 | CCMSLIB00005777178 | CCMSLIB00005777200 | CCMSLIB00000006292 |
| CCMSLIB00005777218 | CCMSLIB00005788026 | CCMSLIB00005879260 | CCMSLIB00006117142 |
| CCMSLIB00006117144 | CCMSLIB00006117146 | CCMSLIB00006117148 | CCMSLIB00006117149 |
| CCMSLIB00006117151 | CCMSLIB00006117153 | CCMSLIB00000006467 | CCMSLIB00006117155 |
| CCMSLIB00006117156 | CCMSLIB00006117158 | CCMSLIB00006117162 | CCMSLIB00006117167 |
| CCMSLIB00006117169 | CCMSLIB00006117171 | CCMSLIB00000006468 | CCMSLIB00006117172 |
| CCMSLIB00006117174 | CCMSLIB00006117176 | CCMSLIB00006117512 | CCMSLIB00006117514 |
| CCMSLIB00006117516 | CCMSLIB00006117518 | CCMSLIB00006117520 | CCMSLIB00006117522 |
| CCMSLIB00006117524 | CCMSLIB00000006469 | CCMSLIB00006117526 | CCMSLIB00006117527 |
| CCMSLIB00006117529 | CCMSLIB00006117531 | CCMSLIB00006117533 | CCMSLIB00006117535 |
| CCMSLIB00006117537 | CCMSLIB00006117539 | CCMSLIB00006117540 | CCMSLIB00006117542 |
| CCMSLIB00000006470 | CCMSLIB00006117544 | CCMSLIB00006117546 | CCMSLIB00006117548 |
| CCMSLIB00006117549 | CCMSLIB00006117551 | CCMSLIB00006117554 | CCMSLIB00006117556 |
| CCMSLIB00006117558 | CCMSLIB00006117559 | CCMSLIB00000006471 | CCMSLIB00006117561 |
| CCMSLIB00006117563 | CCMSLIB00006117564 | CCMSLIB00006117566 | CCMSLIB00004702881 |
| CCMSLIB00004702882 | CCMSLIB00004702883 | CCMSLIB00004702884 | CCMSLIB00004702885 |
| CCMSLIB00004702886 | CCMSLIB00004702887 | CCMSLIB00004702888 | CCMSLIB00004702889 |
| CCMSLIB00000005096 | CCMSLIB00004721125 | CCMSLIB00004721126 | CCMSLIB00000005097 |
| CCMSLIB00004721127 | CCMSLIB00004721131 | CCMSLIB00004721132 | CCMSLIB00004721133 |
| CCMSLIB00004721134 | CCMSLIB00004721135 | CCMSLIB00004721136 | CCMSLIB00004721137 |
| CCMSLIB00004721138 | CCMSLIB00004721139 | CCMSLIB00000005098 | CCMSLIB00004721437 |
| CCMSLIB00004721443 | CCMSLIB00000005099 | CCMSLIB00000005100 | CCMSLIB00000005101 |
| CCMSLIB00000004263 | CCMSLIB00004721937 | CCMSLIB00004721938 | CCMSLIB00004722202 |
| CCMSLIB00005434451 | CCMSLIB00000005102 | CCMSLIB00005434452 | CCMSLIB00005434461 |
| CCMSLIB00005436472 | CCMSLIB00005463708 | CCMSLIB00005489639 | CCMSLIB00005489641 |
| CCMSLIB00005489643 | CCMSLIB00000005103 | CCMSLIB00005489645 | CCMSLIB00005489646 |
| CCMSLIB00005489647 | CCMSLIB00005716834 | CCMSLIB00005716876 | CCMSLIB00005716877 |
| CCMSLIB00005716878 | CCMSLIB00005716879 | CCMSLIB00005716880 | CCMSLIB00005720309 |
| CCMSLIB00005723212 | CCMSLIB00005723213 | CCMSLIB00005723214 | CCMSLIB00005723221 |
| CCMSLIB00005723222 | CCMSLIB00005723223 | CCMSLIB00005723224 | CCMSLIB00005723225 |
| CCMSLIB00005723226 | CCMSLIB00005723233 | CCMSLIB00000005105 | CCMSLIB00005723234 |
| CCMSLIB00005723235 | CCMSLIB00005723236 | CCMSLIB00005723237 | CCMSLIB00005723238 |
| CCMSLIB00005723245 | CCMSLIB00005723246 | CCMSLIB00005723247 | CCMSLIB00005723260 |
| CCMSLIB00005723261 | CCMSLIB00005723262 | CCMSLIB00005723269 | CCMSLIB00005723270 |
| CCMSLIB00005723271 | CCMSLIB00005723275 | CCMSLIB00005723276 | CCMSLIB00005723277 |
| CCMSLIB00005724392 | CCMSLIB00005726900 | CCMSLIB00000005407 | CCMSLIB00005726922 |
| CCMSLIB00005726923 | CCMSLIB00005726980 | CCMSLIB00005726986 | CCMSLIB00005726998 |
| CCMSLIB00005727002 | CCMSLIB00005727028 | CCMSLIB00005727039 | CCMSLIB00005727131 |
| CCMSLIB00000005408 | CCMSLIB00005727285 | CCMSLIB00005727341 | CCMSLIB00005727524 |
| CCMSLIB00005727676 | CCMSLIB00005727888 | CCMSLIB00005727939 | CCMSLIB00005730009 |
| CCMSLIB00005730083 | CCMSLIB00005730138 | CCMSLIB00005730168 | CCMSLIB00005730194 |
| CCMSLIB00005730244 | CCMSLIB00005730299 | CCMSLIB00005730300 | CCMSLIB00005730382 |
| CCMSLIB00005730444 | CCMSLIB00005730462 | CCMSLIB00005730664 | CCMSLIB00005730719 |
| CCMSLIB00005730816 | CCMSLIB00005730881 | CCMSLIB00005730901 | CCMSLIB00005730929 |
| CCMSLIB00005730938 | CCMSLIB00005730953 | CCMSLIB00005730981 | CCMSLIB00005731084 |
| CCMSLIB00000004264 |

Beta-lactams:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005771186 | CCMSLIB00005771194 | CCMSLIB00005771217 | CCMSLIB00005771246 |
| CCMSLIB00005771257 | CCMSLIB00005771277 | CCMSLIB00005771279 | CCMSLIB00005771303 |
| CCMSLIB00005771334 | CCMSLIB00005771340 | CCMSLIB00005771369 | CCMSLIB00005771440 |
| CCMSLIB00005771457 | CCMSLIB00005771474 | CCMSLIB00005771499 | CCMSLIB00005771530 |
| CCMSLIB00005771533 | CCMSLIB00005771586 | CCMSLIB00005772086 | CCMSLIB00005772087 |
| CCMSLIB00005772093 | CCMSLIB00005772109 | CCMSLIB00005772167 | CCMSLIB00005772192 |
| CCMSLIB00005772302 | CCMSLIB00005772340 | CCMSLIB00005772360 | CCMSLIB00005772368 |
| CCMSLIB00005772377 | CCMSLIB00005772391 | CCMSLIB00005772402 | CCMSLIB00005772420 |
| CCMSLIB00005772458 | CCMSLIB00005772539 | CCMSLIB00005772589 | CCMSLIB00005772617 |
| CCMSLIB00005772622 | CCMSLIB00005772687 | CCMSLIB00005772744 | CCMSLIB00005772751 |
| CCMSLIB00005772782 | CCMSLIB00005772869 | CCMSLIB00005772876 | CCMSLIB00005772908 |
| CCMSLIB00005772910 | CCMSLIB00005772945 | CCMSLIB00000005987 | CCMSLIB00005772987 |
| CCMSLIB00005773059 | CCMSLIB00005773135 | CCMSLIB00005773179 | CCMSLIB00005773180 |
| CCMSLIB00005773226 | CCMSLIB00005773275 | CCMSLIB00005773285 | CCMSLIB00005773294 |
| CCMSLIB00005773346 | CCMSLIB00005773456 | CCMSLIB00005773655 | CCMSLIB00005773670 |
| CCMSLIB00005773698 | CCMSLIB00005773712 | CCMSLIB00005773730 | CCMSLIB00005773733 |
| CCMSLIB00005773811 | CCMSLIB00005773954 | CCMSLIB00005773970 | CCMSLIB00005774043 |
| CCMSLIB00005774098 | CCMSLIB00005774106 | CCMSLIB00005774226 | CCMSLIB00005774335 |
| CCMSLIB00005774348 | CCMSLIB00005774403 | CCMSLIB00005774605 | CCMSLIB00005774809 |
| CCMSLIB00005774837 | CCMSLIB00005774859 | CCMSLIB00005774870 | CCMSLIB00005774945 |
| CCMSLIB00005774982 | CCMSLIB00005775055 | CCMSLIB00005775063 | CCMSLIB00005775098 |
| CCMSLIB00005775215 | CCMSLIB00005775227 | CCMSLIB00005775237 | CCMSLIB00005775249 |
| CCMSLIB00000206381 | CCMSLIB00000206437 | CCMSLIB00000206438 | CCMSLIB00000206439 |
| CCMSLIB00000206440 | CCMSLIB00000206441 | CCMSLIB00000206675 | CCMSLIB00000206676 |
| CCMSLIB00000206677 | CCMSLIB00000206678 | CCMSLIB00000206679 | CCMSLIB00000206680 |
| CCMSLIB00000206681 | CCMSLIB00000206682 | CCMSLIB00000206683 | CCMSLIB00000206684 |
| CCMSLIB00000206685 | CCMSLIB00000206686 | CCMSLIB00000206687 | CCMSLIB00000206688 |
| CCMSLIB00000207314 | CCMSLIB00000207316 | CCMSLIB00000207317 | CCMSLIB00000004833 |
| CCMSLIB00000207318 | CCMSLIB00000207319 | CCMSLIB00000207322 | CCMSLIB00000207323 |
| CCMSLIB00000207324 | CCMSLIB00000207327 | CCMSLIB00000004834 | CCMSLIB00000207330 |
| CCMSLIB00000207331 | CCMSLIB00000207336 | CCMSLIB00000207337 | CCMSLIB00000004835 |
| CCMSLIB00000207338 | CCMSLIB00000207342 | CCMSLIB00000207344 | CCMSLIB00000207345 |
| CCMSLIB00000207346 | CCMSLIB00000207347 | CCMSLIB00000004836 | CCMSLIB00000207348 |
| CCMSLIB00000207350 | CCMSLIB00000207351 | CCMSLIB00000207352 | CCMSLIB00000207353 |
| CCMSLIB00000207354 | CCMSLIB00000207355 | CCMSLIB00000207356 | CCMSLIB00000207357 |
| CCMSLIB00000004837 | CCMSLIB00000207358 | CCMSLIB00000207359 | CCMSLIB00000207360 |
| CCMSLIB00000207361 | CCMSLIB00000207362 | CCMSLIB00000207363 | CCMSLIB00000207364 |
| CCMSLIB00000207365 | CCMSLIB00000207366 | CCMSLIB00000207367 | CCMSLIB00000004838 |
| CCMSLIB00000207368 | CCMSLIB00000207369 | CCMSLIB00000207370 | CCMSLIB00000207372 |
| CCMSLIB00000207373 | CCMSLIB00000207374 | CCMSLIB00000207375 | CCMSLIB00000207376 |
| CCMSLIB00000207378 | CCMSLIB00000207379 | CCMSLIB00000207380 | CCMSLIB00000207381 |
| CCMSLIB00000207557 | CCMSLIB00000207559 | CCMSLIB00000207560 | CCMSLIB00000004845 |
| CCMSLIB00000001639 | CCMSLIB00000207561 | CCMSLIB00000207562 | CCMSLIB00000207563 |
| CCMSLIB00000207564 | CCMSLIB00000207565 | CCMSLIB00000207566 | CCMSLIB00000207567 |
| CCMSLIB00000207568 | CCMSLIB00000207569 | CCMSLIB00000207570 | CCMSLIB00000004846 |
| CCMSLIB00000208371 | CCMSLIB00000208372 | CCMSLIB00000208373 | CCMSLIB00000208374 |
| CCMSLIB00000208375 | CCMSLIB00000208376 | CCMSLIB00000208377 | CCMSLIB00000208378 |
| CCMSLIB00000208379 | CCMSLIB00000208380 | CCMSLIB00000004847 | CCMSLIB00000208381 |
| CCMSLIB00000208382 | CCMSLIB00000208383 | CCMSLIB00000208384 | CCMSLIB00000208386 |
| CCMSLIB00000208387 | CCMSLIB00000208632 | CCMSLIB00000004848 | CCMSLIB00000208634 |
| CCMSLIB00000208637 | CCMSLIB00000208638 | CCMSLIB00000208639 | CCMSLIB00000208640 |
| CCMSLIB00000208643 | CCMSLIB00000004849 | CCMSLIB00000208644 | CCMSLIB00000208645 |
| CCMSLIB00000217240 | CCMSLIB00000217242 | CCMSLIB00000217244 | CCMSLIB00000218032 |
| CCMSLIB00000218036 | CCMSLIB00000219036 | CCMSLIB00000004851 | CCMSLIB00000219042 |
| CCMSLIB00000219660 | CCMSLIB00000219662 | CCMSLIB00000219746 | CCMSLIB00000004852 |
| CCMSLIB00000220299 | CCMSLIB00000004871 | CCMSLIB00000220965 | CCMSLIB00000220967 |
| CCMSLIB00000220969 | CCMSLIB00000004872 | CCMSLIB00000221167 | CCMSLIB00000221225 |

Griseofulvins:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00005775327 | CCMSLIB00005775482 | CCMSLIB00005775559 | CCMSLIB00005775608 |
| CCMSLIB00005775616 | CCMSLIB00005775681 | CCMSLIB00000006287 | CCMSLIB00005775786 |
| CCMSLIB00005775821 | CCMSLIB00005775872 | CCMSLIB00005775888 | CCMSLIB00005775898 |
| CCMSLIB00005775916 | CCMSLIB00005775919 | CCMSLIB00000006288 | CCMSLIB00005776075 |
| CCMSLIB00005776103 | CCMSLIB00005776106 | CCMSLIB00005776114 | CCMSLIB00005776174 |
| CCMSLIB00005776191 | CCMSLIB00005776239 | CCMSLIB00005776412 | CCMSLIB00000006289 |
| CCMSLIB00005776414 | CCMSLIB00005776468 | CCMSLIB00005776473 | CCMSLIB00005776515 |
| CCMSLIB00005776520 | CCMSLIB00005776527 | CCMSLIB00005776549 | CCMSLIB00000006290 |
| CCMSLIB00005776581 | CCMSLIB00005776582 | CCMSLIB00005776597 | CCMSLIB00005776639 |
| CCMSLIB00005776652 | CCMSLIB00005776683 |

Indolocarbazoles:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00006117568 | CCMSLIB00006117569 | CCMSLIB00006117571 | CCMSLIB00006117841 |
| CCMSLIB00006117842 | CCMSLIB00006117844 | CCMSLIB00000006472 | CCMSLIB00006117846 |

Lincosamides:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00006117848 | CCMSLIB00006117850 | CCMSLIB00006117852 | CCMSLIB00006117854 |
| CCMSLIB00006117855 | CCMSLIB00006117857 | CCMSLIB00006117860 | CCMSLIB00006117862 |
| CCMSLIB00000006613 | CCMSLIB00006117864 | CCMSLIB00006120790 | CCMSLIB00006120792 |
| CCMSLIB00006120794 | CCMSLIB00006120795 | CCMSLIB00006120797 | CCMSLIB00006120799 |
| CCMSLIB00006120801 | CCMSLIB00006120803 | CCMSLIB00000006614 | CCMSLIB00006120804 |
| CCMSLIB00006120806 | CCMSLIB00006120808 | CCMSLIB00006120809 | CCMSLIB00006120811 |
| CCMSLIB00006581707 | CCMSLIB00006679883 | CCMSLIB00006680141 | CCMSLIB00000006615 |
| CCMSLIB00006684416 | CCMSLIB00006684510 | CCMSLIB00006684585 | CCMSLIB00006684624 |
| CCMSLIB00006685296 | CCMSLIB00006685304 | CCMSLIB00006685311 | CCMSLIB00006718016 |
| CCMSLIB00006718017 | CCMSLIB00006718018 | CCMSLIB00006718028 | CCMSLIB00006718031 |
| CCMSLIB00006718032 | CCMSLIB00008851481 | CCMSLIB00008851484 | CCMSLIB00008851495 |
| CCMSLIB00000006617 | CCMSLIB00008851497 |

Macrolides:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00008851499 | CCMSLIB00009918375 | CCMSLIB00009918376 | CCMSLIB00009918930 |
| CCMSLIB00009918939 | CCMSLIB00009919327 | CCMSLIB00010011918 | CCMSLIB00010013005 |
| CCMSLIB00010013021 | CCMSLIB00000006618 | CCMSLIB00010104431 | CCMSLIB00010105282 |
| CCMSLIB00010105283 | CCMSLIB00010106266 | CCMSLIB00010106267 | CCMSLIB00010107984 |
| CCMSLIB00010108385 | CCMSLIB00010108387 | CCMSLIB00010108639 | CCMSLIB00010108640 |
| CCMSLIB00000006619 | CCMSLIB00010109073 | CCMSLIB00010109074 | CCMSLIB00010109100 |
| CCMSLIB00010109103 | CCMSLIB00010109294 | CCMSLIB00010110459 | CCMSLIB00010110715 |
| CCMSLIB00010110717 | CCMSLIB00010111110 | CCMSLIB00000006620 | CCMSLIB00010111111 |
| CCMSLIB00010111416 | CCMSLIB00010111418 | CCMSLIB00010112253 | CCMSLIB00010112744 |
| CCMSLIB00010113483 | CCMSLIB00010113484 | CCMSLIB00010114019 | CCMSLIB00010114020 |
| CCMSLIB00010114094 | CCMSLIB00010114095 | CCMSLIB00010114360 | CCMSLIB00010114475 |
| CCMSLIB00010115766 | CCMSLIB00010116621 | CCMSLIB00010116622 | CCMSLIB00010117604 |
| CCMSLIB00010117605 | CCMSLIB00010119319 | CCMSLIB00010119722 | CCMSLIB00000006871 |
| CCMSLIB00010119724 | CCMSLIB00010119977 | CCMSLIB00010119978 | CCMSLIB00010120415 |
| CCMSLIB00010120441 | CCMSLIB00010120444 | CCMSLIB00010120635 | CCMSLIB00010120636 |
| CCMSLIB00010121799 | CCMSLIB00010122056 | CCMSLIB00010122058 | CCMSLIB00010122445 |
| CCMSLIB00010122446 | CCMSLIB00010122751 | CCMSLIB00010122753 | CCMSLIB00010124067 |
| CCMSLIB00010124808 | CCMSLIB00010124809 | CCMSLIB00010125344 | CCMSLIB00010125345 |
| CCMSLIB00010125419 | CCMSLIB00010125420 | CCMSLIB00010125687 | CCMSLIB00010125805 |
| CCMSLIB00011427535 | CCMSLIB00011427554 | CCMSLIB00011427556 | CCMSLIB00000075306 |
| CCMSLIB00011429458 | CCMSLIB00011437821 | CCMSLIB00012060397 | CCMSLIB00000075307 |
| CCMSLIB00000075308 | CCMSLIB00000075309 | CCMSLIB00000075310 | CCMSLIB00000075311 |
| CCMSLIB00000075312 | CCMSLIB00000075331 | CCMSLIB00000075332 | CCMSLIB00000076971 |
| CCMSLIB00000076997 | CCMSLIB00000077000 | CCMSLIB00000077001 | CCMSLIB00000077020 |
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| CCMSLIB00000077091 | CCMSLIB00000077092 | CCMSLIB00000077102 | CCMSLIB00000004457 |
| CCMSLIB00000077115 | CCMSLIB00000077122 | CCMSLIB00000077129 | CCMSLIB00000077148 |
| CCMSLIB00000077249 | CCMSLIB00000077250 | CCMSLIB00000077251 | CCMSLIB00000078071 |
| CCMSLIB00000004458 | CCMSLIB00000078072 | CCMSLIB00000078101 | CCMSLIB00000078111 |
| CCMSLIB00000078119 | CCMSLIB00000078125 | CCMSLIB00000078151 | CCMSLIB00000078165 |
| CCMSLIB00000078169 | CCMSLIB00000078170 | CCMSLIB00000078178 | CCMSLIB00000004459 |
| CCMSLIB00000001635 | CCMSLIB00000078196 | CCMSLIB00000078197 | CCMSLIB00000078200 |
| CCMSLIB00000078201 | CCMSLIB00000078217 | CCMSLIB00000078218 | CCMSLIB00000078219 |
| CCMSLIB00000078259 | CCMSLIB00000078270 | CCMSLIB00000078271 | CCMSLIB00000004544 |
| CCMSLIB00000078277 | CCMSLIB00000078289 | CCMSLIB00000078290 | CCMSLIB00000078307 |
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| CCMSLIB00000078480 | CCMSLIB00000078481 | CCMSLIB00000004545 | CCMSLIB00000078482 |
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| CCMSLIB00000078953 | CCMSLIB00000078998 | CCMSLIB00000078999 | CCMSLIB00000079018 |
| CCMSLIB00000079026 | CCMSLIB00000079064 | CCMSLIB00000079152 | CCMSLIB00000004692 |
| CCMSLIB00000079273 | CCMSLIB00000079274 | CCMSLIB00000079275 | CCMSLIB00000080629 |
| CCMSLIB00000081287 | CCMSLIB00000084767 | CCMSLIB00000084786 | CCMSLIB00000084864 |
| CCMSLIB00000004693 | CCMSLIB00000084918 | CCMSLIB00000084919 | CCMSLIB00000085015 |
| CCMSLIB00000085023 | CCMSLIB00000085226 | CCMSLIB00000085392 | CCMSLIB00000085443 |
| CCMSLIB00000085464 | CCMSLIB00000085478 | CCMSLIB00000085509 | CCMSLIB00000004694 |
| CCMSLIB00000085510 | CCMSLIB00000085594 | CCMSLIB00000085629 | CCMSLIB00000085633 |
| CCMSLIB00000085751 | CCMSLIB00000085752 | CCMSLIB00000085794 | CCMSLIB00000085880 |
| CCMSLIB00000085918 | CCMSLIB00000085951 | CCMSLIB00000004731 | CCMSLIB00000085983 |
| CCMSLIB00000085990 | CCMSLIB00000086004 | CCMSLIB00000086045 | CCMSLIB00000086123 |
| CCMSLIB00000086151 | CCMSLIB00000086157 | CCMSLIB00000086191 | CCMSLIB00000204903 |
| CCMSLIB00000205615 | CCMSLIB00000004732 | CCMSLIB00000205757 |

Monobactams:

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| --- | --- | --- | --- |
| CCMSLIB00000206304 | CCMSLIB00000206305 | CCMSLIB00000206306 | CCMSLIB00000206363 |
| CCMSLIB00000206364 | CCMSLIB00000001637 | CCMSLIB00000206365 | CCMSLIB00000206366 |
| CCMSLIB00000206378 | CCMSLIB00000206379 | CCMSLIB00000206380 |

Peptides:

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| --- | --- | --- | --- |
| CCMSLIB00000221250 | CCMSLIB00000221359 | CCMSLIB00000221365 | CCMSLIB00000222297 |
| CCMSLIB00000222299 | CCMSLIB00000222301 | CCMSLIB00000004873 | CCMSLIB00000001651 |
| CCMSLIB00000222303 | CCMSLIB00000222308 | CCMSLIB00000222310 | CCMSLIB00000223491 |
| CCMSLIB00000223492 | CCMSLIB00000223493 | CCMSLIB00000223494 | CCMSLIB00000223724 |
| CCMSLIB00000223725 |

Polyenes:

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| CCMSLIB00000223726 | CCMSLIB00000223727 | CCMSLIB00000223746 | CCMSLIB00000223747 |
| CCMSLIB00000223876 | CCMSLIB00000223879 | CCMSLIB00000223998 | CCMSLIB00000004876 |
| CCMSLIB00000424805 | CCMSLIB00000424806 | CCMSLIB00000424807 | CCMSLIB00000424808 |
| CCMSLIB00000427286 | CCMSLIB00000429792 | CCMSLIB00000429794 | CCMSLIB00000478123 |
| CCMSLIB00000478560 | CCMSLIB00000478607 | CCMSLIB00000479755 | CCMSLIB00000479756 |
| CCMSLIB00000479757 | CCMSLIB00000479758 | CCMSLIB00000479767 | CCMSLIB00000479778 |
| CCMSLIB00000531508 | CCMSLIB00000562755 | CCMSLIB00000562760 | CCMSLIB00000562773 |
| CCMSLIB00000562787 | CCMSLIB00000563635 | CCMSLIB00000566026 | CCMSLIB00000566393 |
| CCMSLIB00000566406 | CCMSLIB00000566427 |

Polyether Ionophores:

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| CCMSLIB00000206021 | CCMSLIB00000206022 | CCMSLIB00000206023 | CCMSLIB00000004733 |
| CCMSLIB00000206024 | CCMSLIB00000206025 | CCMSLIB00000206302 | CCMSLIB00000206303 |
| CCMSLIB00000566445 | CCMSLIB00000004879 | CCMSLIB00000566527 | CCMSLIB00000566567 |
| CCMSLIB00000566568 | CCMSLIB00000566571 | CCMSLIB00000566574 | CCMSLIB00000566590 |
| CCMSLIB00000566702 | CCMSLIB00000566729 | CCMSLIB00000566825 | CCMSLIB00000566867 |
| CCMSLIB00000566923 | CCMSLIB00000566936 | CCMSLIB00000566960 | CCMSLIB00000567027 |
| CCMSLIB00000567062 | CCMSLIB00000567077 | CCMSLIB00000567272 | CCMSLIB00000567285 |
| CCMSLIB00000567286 | CCMSLIB00000567313 | CCMSLIB00000567466 | CCMSLIB00000567576 |
| CCMSLIB00000567594 | CCMSLIB00000568417 | CCMSLIB00000568437 | CCMSLIB00000568580 |
| CCMSLIB00000568607 | CCMSLIB00000568610 | CCMSLIB00000568615 | CCMSLIB00000568653 |
| CCMSLIB00000568670 | CCMSLIB00000568691 | CCMSLIB00000568794 |

Surugamides:

|  |  |  |  |
| --- | --- | --- | --- |
| CCMSLIB00000568853 | CCMSLIB00000569054 | CCMSLIB00000569062 | CCMSLIB00000569077 |
| CCMSLIB00000569106 | CCMSLIB00000569117 | CCMSLIB00000569130 |

Tetracyclines:

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| --- | --- | --- | --- |
| CCMSLIB00000004919 | CCMSLIB00000001653 | CCMSLIB00000569139 | CCMSLIB00000569143 |
| CCMSLIB00000569157 | CCMSLIB00000569164 | CCMSLIB00000569170 | CCMSLIB00000569241 |
| CCMSLIB00000569688 | CCMSLIB00000569815 | CCMSLIB00000569920 | CCMSLIB00000004920 |
| CCMSLIB00000570395 | CCMSLIB00000571792 | CCMSLIB00000572468 | CCMSLIB00000572620 |
| CCMSLIB00000572727 | CCMSLIB00000572730 | CCMSLIB00000572744 | CCMSLIB00000572787 |
| CCMSLIB00000572998 | CCMSLIB00000573355 | CCMSLIB00000574193 | CCMSLIB00000574379 |
| CCMSLIB00000577568 | CCMSLIB00000578442 | CCMSLIB00000578443 | CCMSLIB00000579271 |
| CCMSLIB00000579592 | CCMSLIB00000579675 | CCMSLIB00000579702 | CCMSLIB00000579711 |
| CCMSLIB00000579731 | CCMSLIB00000579765 | CCMSLIB00000579885 | CCMSLIB00000579894 |
| CCMSLIB00000839197 | CCMSLIB00000839203 | CCMSLIB00000839204 | CCMSLIB00000839205 |
| CCMSLIB00000839206 | CCMSLIB00000839969 | CCMSLIB00000839970 | CCMSLIB00000839971 |
| CCMSLIB00000840417 | CCMSLIB00000840420 | CCMSLIB00000840421 | CCMSLIB00000840440 |
| CCMSLIB00000841737 | CCMSLIB00000841745 | CCMSLIB00000841825 | CCMSLIB00000841882 |
| CCMSLIB00000841898 | CCMSLIB00000841916 | CCMSLIB00000841921 | CCMSLIB00000841930 |
| CCMSLIB00000851861 | CCMSLIB00000856076 | CCMSLIB00001058581 | CCMSLIB00001058605 |
| CCMSLIB00001058864 | CCMSLIB00001058891 | CCMSLIB00001059048 | CCMSLIB00003134545 |
| CCMSLIB00003134635 | CCMSLIB00003134739 | CCMSLIB00003134743 | CCMSLIB00003134958 |
| CCMSLIB00003134964 | CCMSLIB00003134981 | CCMSLIB00003135180 | CCMSLIB00003135217 |
| CCMSLIB00003135296 | CCMSLIB00003135533 | CCMSLIB00003135571 | CCMSLIB00003135623 |
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| CCMSLIB00003136296 | CCMSLIB00003136327 | CCMSLIB00003136354 | CCMSLIB00000005024 |
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| CCMSLIB00003137135 | CCMSLIB00003137167 | CCMSLIB00003137197 | CCMSLIB00003137264 |
| CCMSLIB00003137289 | CCMSLIB00003137653 | CCMSLIB00003138050 | CCMSLIB00003138082 |
| CCMSLIB00003138099 | CCMSLIB00003138124 | CCMSLIB00003138151 | CCMSLIB00003138467 |
| CCMSLIB00003138470 | CCMSLIB00003138539 | CCMSLIB00003138561 | CCMSLIB00003138564 |
| CCMSLIB00003138587 | CCMSLIB00003138877 | CCMSLIB00003138916 | CCMSLIB00003138994 |
| CCMSLIB00000005027 | CCMSLIB00003139115 | CCMSLIB00003139293 | CCMSLIB00003139459 |
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| CCMSLIB00004693957 | CCMSLIB00004693958 | CCMSLIB00004693959 | CCMSLIB00004693960 |
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| CCMSLIB00004693977 | CCMSLIB00004693978 | CCMSLIB00000005091 | CCMSLIB00000001672 |
| CCMSLIB00004693979 | CCMSLIB00004694115 | CCMSLIB00004694116 | CCMSLIB00004694117 |
| CCMSLIB00004694217 | CCMSLIB00004694218 | CCMSLIB00004694219 | CCMSLIB00004694442 |
| CCMSLIB00004694443 | CCMSLIB00004694444 | CCMSLIB00000005092 | CCMSLIB00000005093 |

Tetramates:

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| CCMSLIB00000005094 | CCMSLIB00004702798 | CCMSLIB00004702878 | CCMSLIB00004702879 |
| CCMSLIB00004702880 |